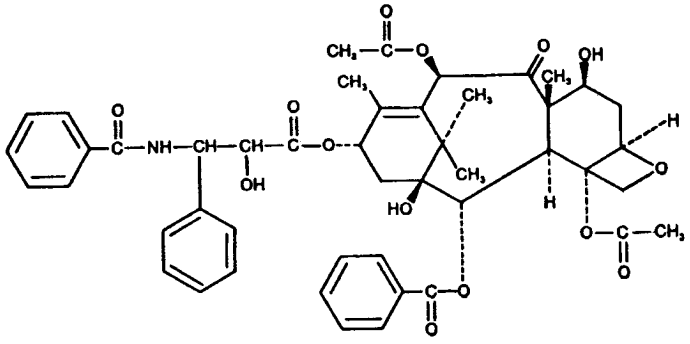
TAXOL

NSC - 125973



Chemical Name: β-(Benzoylamino)-α-hydroxybenzenepropanoic acid, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, [*2aR*-[*2aα,4β,4aβ,6β,9α(αR*,βS*),11α,12α,12aα,12bα*]]-

CAS Registry Number: 33069-62-4

Molecular Formula: $C_{47}H_{51}NO_{14}$ **M.W.:** 853.9

Qualitative Solubility:

Highly insoluble in water and aqueous solvents. Compound dissolves in methanol, ethanol, benzene, chloroform, methylene chloride, and tetrahydrofuran.

Stability:

Bulk:
Bulk samples stored at room temperature for 30 days showed no decomposition as indicated by UV absorption, TLC, or HPLC. The bulk compound stored at 60 °C for three weeks also showed no decomposition. After four weeks very minor decomposition was detected by TLC.

Ultraviolet Absorption:

(MeOH)

λ_{max} = 227 ± 2nm ε = 28,500 - 30,900

High Performance Liquid Chromatography:

Column:	IBM ODS, 5 μm, 4.6 x 250 mm
Mobile Phase:	63% MeOH/37% water
Flow Rate:	1.0 mL/min
Detection:	UV at 230 nm
Sample Preparation:	Dissolve ≈6 mg sample in 10 mL methanol. Mix 1 mL of this solution with 1 mL of internal standard solution.
Internal Standard:	20 mg Paraben in 25 mL methanol
Retention Volume:	19.3 mL (NSC - 125973) 7.7 mL (I.S.)

Optical Rotation:

(c = 1, MeOH) $[\alpha]_D^{20} = -53 \pm 2°$

Toxicity Data:

Rat(ip): LD_{50}: 32530 μg/kg
National Technical Information Service, PB83-170969

Mouse(ip): LD_{50} 128 mg/kg
National Technical Information Service, PB83-170969

Dog(iv): LD_{50}: 15 mg/kg
National Technical Information Service, PB83-170969